SUBJECT INDEX

Acetylene 466
Adamantanes 450–1
ADC (apparent diffusion coefficient) 114
Aliphatic compounds, open-chain 416–21
Alkenes, carbon–carbon coupling constants 451–65
Alkynes, carbon–carbon coupling constants 466–70
Al_2O_3 surface OH groups, interaction with V_2O_5 286–7
Alternate delay accumulation 146
Alumina, ^1H NMR spectra 267–8
Aluminophosphate catalysts 271–2
Amides 545–55
Amines 545–55
Aminoacids, carbon–carbon coupling constants 571–9
Amplitude correction 180
Analog-to-digital converter (ADC) 140, 218
Angiography. *See* MR angiography
Apodization 219–22
Aromatic compounds, carbon–carbon coupling constants 470–523
Artifact reduction 105
Artifact sources 105
Artificial intelligence 232
Auto-tracer methods 124
Azines 532–6
Azo-compounds 555–9
Azoles 525
Azoxy-compounds 555–9
Azulene derivatives, carbon–carbon coupling constants 517–23

Baseline correction 179, 218
Baseline quality factor 177
BASIS 233
Bayesian analysis 227
Benzene derivatives, carbon–carbon coupling constants 470–96
Bicyclo[2.2.2]octanes 448–9
Bicycloalkanes 429–51
Bicyclo[*n*.1.1]alkanes 442–5
Bicycloalkenes 464–5
Bicyclobutanes 429
Binomial preparation process 193–4
Binomial refocusing 191
Binomial sequences 156–9
Biological species, carbon–carbon coupling constants 571–95
Biosynthetic metabolites and by-products, carbon–carbon coupling constants 593–5
Bipolar gradient pulses 97
Black-blood methods 107–10
Bloch equations 143, 148–9
Bloch spins 143–5, 148–9
Bolus tracking 102–3

Caged carbocyclic compounds 429–51
Carbenium ions 569–71
Carbohydrates, carbon–carbon coupling constants 579–93
Carbon–carbon coupling constants 301–610
  additivity 406–14
  alkenes 451–65
  alkynes 466–70
  aminoacids 571–9
  aromatic compounds 470–523
  azulene derivatives 517–23
  benzene derivatives 470–96
  bicycloalkanes, caged carbocyles and related systems 429
  biological species 571–95
  biosynthetic metabolites and by-products 593–5
  bond angle dependences 359–60
  carbohydrates 579–93
  charged systems 569–71
  condensed aromatics 496–517
  determination of signs 323–33
  dihedral angle dependences 360–71
  elemento-organic compounds 564–8
  empirical and theoretical treatments 336–416
  experimental techniques 302–23
  geminal couplings 371
  general trends 336–9
  heteroatomic bridge transmission 414
  heterocyclic compounds 523–37
  hetroatomic compounds 537–64
  hybridization 339–42
  lone pair effects 386–95
  medium effects 414–16
  metallo-organic compounds 564–8
  multipath coupling mechanism 410–14
  non-benzenoid aromatics 517–23
  open-chain aliphatic compounds 416–21
  orientation of terminal substituent 371–6
  peptides 571–9
  saturated compounds 416–51
  stereochemical applications 395–406
  steric effects 359–406
  substituent effects 342–59
  theory and computation 333–6
  through-space and non-bonded interactions 376–86
  vicinal couplings 371–6
Carbonyl containing compounds 537–41
Catalyst in sealed sample tubes 262–3

Cathode ray oscilloscope (CRO) 245
C_6D_6 273
CH_3OH
  adsorption complexes on zeolites 296–7
  catalytic reaction with H_2S 295–6
Charged heteroaromatics 571
Charged systems, carbon–carbon coupling constants 569–71
Chemical shifts 247
  interaction 6–7
  surface OH groups 263–6
  zeolite catalysts 263–6
CHEMICS 233
Combined (sample) rotation and multiple-pulse spectroscopy (CRAMPS) 24–5
Computer hardware 253–4
Computing resources 214
Condensed aromatics, carbon–carbon coupling constants 496–517
Constant-phase response 153
Constant time imaging 8–11
Convolution back projection 11–12
CRAMPS 38, 261
Cubanes 449–50
Cubic spline 245
Curve fitting techniques 229–31
CW-NMR 212
Cycloalkenes 459–62
Cyclobutanes 427–8
Cyclohexanes 428–9
Cyclopentanes 428–9
Cyclopropanes 421–7

Data acquisition 140
Data evaluation 211–58
Data processing 211–58
  effect on NMR data structure 252
  future developments 253
  history 212–14
  methods 214–34
Data shift accumulation 146
Data structure 252
Data visualization 234–52
DENDRAL 233
Dependent variable (intensity) representation 234–7
Deuterated tracers 126
Diamantanes 450–1
Diffusion gradients 118
Dilute spins imaging by polarisation transfer 28–33
Dipole–dipole interaction 4–6
Discrete fourier transform (DFT) 224
DISPA plot 229
Dy-DTPA 122
Dynamic nuclear polarisation (DNP) 31

Echo excitation sequence 166
Echo-planar imaging (EPI) 110, 121
Echo-planar single-shot diffusion imaging 115–17
Elemento-organic compounds, carbon–carbon coupling constants 564–8
ERASER 168
Esters 542–5
Ethers 542–5
Excitation sequence 159
  duration of 177
  relaxation during 148
Excitation spectrum 145
  frequency-dependent phase shift of 149–51
EXORCYCLE 166, 167, 187
Expert systems 232–4, 254–5

Field modulating 28
FLASH 121, 122
Flow compensation by gradient moment nulling 97–8
Flow encoding 97
Flow imaging *in vivo* 94–5
Flow mapping 102
Flow zeugmatography 98
Fluorinated tracers 125
4D $^{13}C/^{13}C$-edited NOESY experiment 84–90
4D $^{13}C/^{15}N$-edited NOESY experiment 82–4
Fourier flow imaging 118
Fourier transform 224
Framework 245–50
Free induction decay (FID) 8, 179, 212, 218–20, 223–5, 228, 247
Free precession acquisition 140–2
Frequency-dependent phase shift of excitation spectrum 149–51
Frequency domain conversion 224
Frequency domain processing 228–34
Frequency-selective E1 excitation 192–3
FT-NMR 212, 214, 224, 228

Gd-DTPA 122
Gd-DTPA-albumen 121
Gradient isocentre (GI) 25
Gradient moment nulling 97–8
Gradient system 36–7
Graphics hardware 251–2
Graphics screens 251–2
GRASS 121, 122

^1H NMR MAS spectroscopy 259–99
  adsorbed molecules 287–97
  catalysts in sealed sample tubes 262–3
  general considerations 260–2
  surface OH groups 263–76
Hard-pulse E1 excitation 191–2
Hardcopy output 252
Hartman–Hahn matching condition 29
H–D exchange 273
Heteroatomic compounds, carbon–carbon coupling constants 537–64
Heterocyclic compounds, carbon–carbon coupling constants 523–37
Heterogeneous catalysis 259–99

Heterogeneous catalysts, commonly used supports for 266–70
Heteronuclear 3D NMR 46–7
  assignment of spin systems by 53–65
  building blocks of 47–50
  conventional sequential assignment using 65–8
  sequential assignment using 53–74
Heteronuclear 3D NMR experiments 75–9
Heteronuclear 4D NMR 46–7, 79–90
  building blocks of 47–50
Heteronuclear multiple quantum coherence (HMQC) building block 47
Homonuclear 3D NMR 46
Homo-spoil 166, 184–5
HOSE 233
$H_3PW_{12}O_{40}$ supported on SiO_2 277–9
H_2S, catalytic reaction with CH_3OH 295–6
Hue lightness saturation (HLS) 236
Hybridization of coupled carbons 339–42
Hydrogen sulfide adsorption on heterogeneous catalysts 291–4
Hypersurface fitting 229–31
H-ZSM-5 zeolite 273, 296–7

Imino-compounds 555–9
Independent variable axes 234
INEPT building block 47
INEPT transfer 47, 49
Interpolation 245
Intra-voxel coherent motion (IVCM) imaging 118–20
Intra-voxel incoherent motion (IVIM) 111, 119–20
Inversion recovery variant of echo-planar imaging (IR-EPI) 122
In vivo localized spectroscopy, specificity of 185–6

J couplings, one-bond and two-bond 68–74
Jeener–Broekaert echo 11
JR-based alternative 167–8
Jump and return (JR) 160–2, 180

Lactams 545–55
Lactones 542–5
Lee–Goldburg method 25–8
Levenberg–Marquardt algorithm 212, 230
Line broadening mechanisms 4–7
Linear approximation 148–9, 155–6
Linear prediction (LP) 212, 227–8
Linear responses 145
Localized excitation methods 186–7
Long-pulse suppression methods 155–6
Long pulses 196

Magic angle concept 25–8
Magic angle spinning (MAS) 20–5. *See also* ^1H NMR MAS
Magnetic moment 138
Maximum entropy method (MEM) 212, 225–7
Maximum likelihood method (MLM) 213, 227
Metallo-organic compounds, carbon–carbon coupling constants 564–8
Methylenebenzocycloalkanes 462–4
Methylenebicycloalkanes 464–5
Methylenecycloalkanes 459–62
Minimum area reconstruction of spectra (MARS) 227
Mixed excitation 184–5
Modified binomials 164–6
Molecular modeling 255
MoO_3/γ-Al_2O_3 catalysts 281–2
MoO_3/SiO_2 catalysts 282–3
MR angiography 96–110
  classification of methods 96
  current technology 96–7
  display post-processing 96–7
  phase effects 97–102
  time-of-flight 102–10
MREV-8 cycle 14–17, 19
Multi-dimensional NMR
  basic principles 44–52
  experimental considerations 50–2
Multiple-phase methods 13–20
Multiple-quantum coherence imaging 33–4
Multipulse spin-echo diffusion imaging 112–15

NERO sequences 167–8
Networking 214, 254
Nitrogen containing compounds 545–55
NMR tracer methods 124
Non-benzenoid aromatics, carbon–carbon coupling constants 517–23
Non-linear effects 156
Non-linear response 148–9
Norbornanes 446–8
Norcubanes 449–50
Nuclear magnetic resonance (NMR) imaging, solid state. *See* Solid state imaging hardware; Solid state imaging methods

Off-resonance excitation pulses 52
OH groups. *See* Surface OH groups
One-dimensional FT–NMR 245
One-dimensional NMR spectra 213
Oxygen containing compounds 542–5
Oxygen-17 tracer 127–8

Peak labels 250
Peptides, carbon–carbon coupling constants 571–9
Perfusion
  concept of 95–6
  dynamic contrast agent studies 120–3
  maps 118
  measurements 111–28
Phase contrast angiography 98–102
Phase corrections 51, 228

Phase cycling 52, 178
Picolines 532–6
Point-resolved spectroscopy (PRESS) 188
Power-adapted JR (PJR) 162–3, 180
Power dissipation 195
Pre-saturation methods 195–6
Primary reference standards 247
Principle component analysis (PCA) 231
Probes 35–6
Projections 237–45
[1.1.1]propellane 442
Propylene adsorption on b-Al_2O_3 288–91
Protein structure determination 43–92
Pseudo-diffusion coefficient 111
Pseudo-diffusion methods 111
Pulse sequences 158
Pulsed gradients 166
Pyridines 532–6

Quadrature detection in indirectly detected dimensions 50
Quadrupole interaction 7

Radiation damping 142, 170
Radio-frequency field inhomogeneity 170
Radio-frequency gradients 187
Raster printer/plotters 252
Receiver system 36
Reduced adjacency matrix (RAM) method 234
Refocused gradient imaging (RGI) techniques 17
Relaxation effects 170
Relaxation measurements 250
Reversed effective field sequences 17–18
Rolling baseline 151–3
Rotating frame 138
Rotating-frame magic angle 25–8

Saturation of water signal in inhomogeneous RF field 188–90
Saturative suppression 104–5
Second averaging applications 19–20
Second order jump and return (SJR) 163
Secondary reference standards 247
Selective and non-selective sub-sequences 159–60, 168
Selective excitation in 2D NMR 184
Selective π pulse sequences 184
Selective spin imaging 28
Self-refocused binomials 164–6
Sensitivity factor 176
Sequential multiple slab 3D acquisition 107
Short pulses 156–9, 196
Signal averager 36
Signal processing 143
Signal-to-noise ratio (SNR) 140
Silica
  ^{1}H NMR spectra 266–7
  modified 273–5
Silicates, ^{1}H NMR spectra 266–7
Simple phase encode method 8
Single long pulse method 137–8, 155–6
Single quantum coherences (SQCs) 33
Solid echo method 8–11
Solid state imaging hardware 35–8
Solid state imaging methods 7–34
Solvent magnetization 153–5
Solvent signal suppression (SSS) 135–209
  data processing 178–81
  effect of fluctuations 172–5
  evaluation criteria 169–78
  excitation, secondary effects of 175–6
  excitation schemes 153–69
  for *in vivo* localized spectroscopy 185–97
  in 1D NMR 181–2
  in 2D and 3D NMR 182–5
  longitudinal magnetization 153
  methods for 137
  review 139
  simulation and subtraction 180
  spectrometer imperfections 171–5
  spectrometer requirements 171–5
  theory 143–53
  transverse magnetization 153
Solvent signal suppression (SSS) factor 169, 170, 176
Spectra imperfections 228
Spectral factor 177
Spin-echo sequences with localization by inhomogeneous RF field 190–4
Spin–spin coupling constants between carbons. *See* Carbon–carbon coupling constants
Spin systems using heteronuclear 3D NMR 53–65
Spurious signals 177
Standard reference compounds 247
Static field inhomogeneity 170–1
Stationary spins 104
Steady-State Free Precession (SSFP) method 107–10
Stejskal–Tanner diffusion gradients 113
STRAY field imaging (STRAFI) 11, 38
Subtractive suppression 104
Sulfides 559–64
Sulfones 559–64
Sulfoxides 559–64
Sulfur containing compounds 559–64
Supported catalysts, active component in 276–81
Surface coils 186, 187
Surface fitting 229–31
Surface OH groups
  chemical shifts 263–6
  1H NMR MAS spectroscopy 263–76

Tagging 104
3D ^{1}H-^{13}C ROESY–HMQC experiment 77
3D ^{1}H-^{15}N HMQC–NOESY–HMQC experiment 77–9
3D ^{1}H-^{15}N HOHAHA–HMQC experiment 53–6
3D ^{1}H-^{15}N ROESY–HMQC experiment 75–6

3D HCACO experiment 73–4
3D H(CA)NH experiment 56–8
3D HCCH–COSY experiment 60–5
3D HCCH–TOCSY experiment 60–5
3D HNCA experiment 58–9
3D HNCO experiment 71–2
3D phase contrast angiography 100
3D (volumetric) acquisition 105
Time domain conversion 224
Time domain processing 218–28
Time-of-flight angiographic methods 104
Time proportional phase incrementation (TPPI) 33, 50, 225
Time reversal by added FIDs (TRAF) functions 212
TiO_2 surface OH groups, interaction with V_2O_5 286–7
Titania, ^1H NMR spectra 268–70
Transform-of-reverse-added-FIDs (TRAF) functions 221–2
Transient B_0 gradients 194–5
Transient gradients 188
Transmitters 35
Travelling presaturation for 2D acquisition 107
Tree diagrams 250
Truncated exponentials
  as base 147–8
  as eigenfunctions 146–7
Truncated response 144, 145, 160
Turbo-FLASH 117
Turbo-STEAM 117
Two-dimensional FT-NMR 245
Two-dimensional heteronuclear multiple quantum coherence NMR (HMQC) 184
Two-dimensional NMR 213, 229, 232
Two-dimensional (sequential slice) acquisition 105–6

Ultra-high intensity grinding 286–7

Velocity density imaging (VDI) method 118–20
Velocity measurement by phase imaging 102
VIGRE (velocity-encoded gradient echoes) 102
V_2O_5, interactions of Al_2O_3 and TiO_2 surface OH groups with 286–7
V_2O_5/SnO_2 catalysts 284–5
V_2O_5/TiO_2 catalysts 285
Volume selection methods 186

WO_3/SiO_2 catalysts 282–3

Zeolite catalysts, chemical shifts 263–6
Zeolites
  adsorption complexes of CH_3OH on 296–7
  surface OH groups in 275–6
Zero filling 223
Z-filter 185
Zirconium hydrides 279–81

CONTENTS OF PREVIOUS VOLUMES

Volume 16

Non-Biological Aspects of Phosphorus-31 NMR Spectroscopy
D. G. GORENSTEIN
Practical Aspects of Tritium Magnetic Resonance
J. P. BLOXSIDGE and J. A. ELVIDGE
The Problem of Intramolecular Rotation in Liquids and Nuclear Magnetic Relaxation
H. G. HERTZ
Product Operator Formalism for the Description of NMR Pulse Experiments
O. W. SØRENSEN, G. W. EICH, M. H. LEVITT, G. BODENHAUSEN and R. R. ERNST
Carbon-13 Chemical Shift Anisotropy
W. S. VEEMAN
Nuclear Magnetic Resonance Studies of Zeolites
J. KLINOWSKI
Multipulse NMR in Liquids
C. J. TURNER

Volume 17

Investigation of the Solution Structures of Short Nucleic Acid Fragments by Means of Nuclear Overhauser Enhancement Measurements
ANGELA M. GRONENBORN and G. MARIUS CLORE
Applications for Dynamic Nuclear Polarization in ^{13}C NMR in Solids
R. A. WIND, M. A. DUIJVESTIJN, C. VAN DER LUGT, A. MANENSCHIJN and J. VRIEND
Steady-State Techniques for Low Sensitivity and Slowly Relaxing Nuclei
A. SCHWENK
Theory of Nuclear Spin Relaxation in Paramagnetic Systems in Solution
J. KOWALEWSKI, L. NORDENSKIÖLD, N. BENETIS and P.-O. WESTLUND
Measuring and Imaging of Flow by NMR
J. STEPIŠNIK
Multipulse Dynamic NMR of Liquid Crystal Polymers
K. MÜLLER, P. MEIER and G. KOTHE
NMR and Compartmentation in Biological Tissues
P. S. BELTON and R. G. RATCLIFFE
Basic Two-Dimensional NMR
D. L. TURNER

Volume 18

^{13}C NMR of Enzymes
J. P. G. MALTHOUSE
Composite Pulses
M. H. LEVITT

NMR-Studies of Phosphoryl Transferring Enzymes
P. RÖSCH
NMR Field-Cycling Spectroscopy: Principles and Applications
F. NOACK
Measurement of Spin Coupling Constants to Quadrupolar Nuclei via Relaxation Studies
V. MLYNÁRIK
^{13}C-NMR Spectral Studies of the N-Terminal Portion of Glycophorins
K DILL and R. D. CARTER
New Developments in NMR of Simple Electrolyte Solutions
M. HOLZ

Volume 19

Fourier Transform Pulsed-Gradient Spin-Echo Studies of Molecular Diffusion
P. STILBS
Broadband Spin Decoupling in Isotropic Liquids
A. J. SHAKA and J. KEELER
Carbon-13 NMR Spectroscopy of Cardenolides and Bufadienolides
W. ROBIEN, B. KOPP, D. SCHABL and H. SCHWARZ
Applications of NMR Methods to the Physical Chemistry of Micellar Solutions
C. CHACHATY
Theoretical and Practical Aspects of One- and Two-dimensional Heteronuclear Overhauser Experiments and Selective ^{13}C T_1-Determinations of Heteronuclear Distances
K. E. KÖVÉR and G. BATTA
Methods of Avoiding the Effects of Acoustic Ringing in Pulsed Fourier Transform Nuclear Magnetic Resonance Spectroscopy
I. P. GEROTHANASSIS
White Noise Nonlinear System Analysis in Nuclear Magnetic Resonance Spectroscopy
B. BLÜMICH

Volume 20

2D NMR Applied to Dynamic Stereochemical Problems
R. WILLEM
Application of ^{1}H, ^{13}C and ^{15}N NMR in the Chemistry of 1,4-Diazines
O. N. CHUPAKHIN, V. N. CHARUSHIN and A. I. CHERNYSHEV
Isotope Effects in Nuclear Shielding
P. E. HANSEN
NMR Methods for Measuring Enzyme Kinetics *in vivo*
K. M. BRINDLE
The Superspin Formalism for Pulse NMR
A. D. BAIN
Optimal Design of Relaxation Time Experiments
G. H. WEISS and J. A. FERRETTI
^{13}C Labeling in Studies of Metabolic Regulation
R. E. LONDON

The Tube Concept of Macromolecular Liquids in the Light of NMR Experiments
R. KIMMICH, G. SCHNUR and M. KÖPF
Thallium NMR Spectroscopy
J. F. HINTON, K. R. METZ and R. W. BRIGGS
Linear Prediction and Maximum Entropy Methods in NMR Spectroscopy
D. S. STEPHENSON

Volume 21

Multinuclear Studies of Aluminium Compounds
J. W. AKITT
Displacive Order–Disorder Crossover in Perovskite and Antifluorite Crystals Undergoing Rotational Phase Transitions
R. L. ARMSTRONG
Orientation of the Rotational Diffusion Principal Axis System Determined by Nuclear Relaxation Data
A. DÖLLE and T. BLUHM
Quadrupolar Relaxation and Thermodynamical Processes in Liquid Metallic Alloys
K. OTT, M. A. HAGHANI, C. A. PAULICK and D. QUITMANN
Construction, Evolution and Detection of Magnetization Modes Designed for Treating Longitudinal Relaxation of Weakly Coupled Spin 1/2 Systems with Magnetic Equivalence
D. CANET
Structural Applications of One-Bond Carbon–Carbon Spin–Spin Coupling Constants
L. B. KRIVDIN and G. A. KALABIN
High Resolution Proton Magnetic Resonance Spectroscopy of Biological Fluids
J. K. NICHOLSON and I. D. WILSON
Polarization Transfer Experiments in High-Resolution NMR Spectroscopy
O. W. SØRENSEN

Volume 22

Scaling in One and Two Dimensional NMR Spectroscopy in Liquids
R. V. HOSUR
Oligosaccharide Conformations: Application of NMR and Energy Calculations
S. W. HOMANS
Relaxation Matrix Analysis of 2D NMR Data
B. A. BORGIAS, M. GOCHIN, D. J. KERWOOD and T. L. JAMES
NMR Investigations of Protein Structure
G. WAGNER
Quantitative Investigations of Molecular Stereodynamics by 1D and 2D NMR Methods
K. G. ORRELL, V. ŠIK and D. STEPHENSON
NMR Parameters of Alkynes
B. WRACKMEYER and K. HORCHLER
Improved Methods for Quantitative Spectral Analysis of NMR Data
H. GESMAR, J. J. LED and F. ABILDGAARD

^{29}Si NMR Spectroscopy of Trimethylsilyl Tags
J. SCHRAML
Primary and Secondary Structures of Synthetic Polymer Systems as Studied by ^{13}C NMR Spectroscopy
I. ANDO, T. YAMANOBE and T. ASAKURA
Solid State NMR Techniques for the Study of Surface Phenomena
J.-PH. ANSERMET, C. P. SLICHTER and J. H. SINFELT
A Primer on Isotopic Labeling in NMR Investigations of Biopolymers
P. H. BOLTON
Vanadium-51 NMR
O. W. HOWARTH
Field-Cycling Relaxometry of Protein Solutions and Tissue: Implications for MRI
S. H. KOENIG and R. D. BROWN III
Solid State NMR Studies of Local Motions in Polymers
A. K. ROY and P. T. INGLEFIELD